2-Chloro-N-methylacetamide

Other names:	Acetamide, 2-chloro-N-methyl-
	N-Methyl-2-chloroacetamide
	N-Methylchloroacetamide
	USAF DO-35
	«alpha»-Chloro-N-methylacetamide
	ClCON(CH3)2
Inchi:	InChI=1S/C3H6ClNO/c1-5-3(6)2-4/h2H2,1H3,(H,5,6)
InchiKey:	HOZLOOPIXHWKCI-UHFFFAOYSA-N
Formula:	C3H6ClNO
SMILES:	CNC(=O)CCl
Mol. weight [g/mol]:	107.54
CAS:	96-30-0

Physical Properties

Property code	Value	Unit	Source
affp	845.80	kJ/mol	NIST Webbook
basg	814.80	kJ/mol	NIST Webbook
gf	-77.08	kJ/mol	Joback Method
hf	-180.10	kJ/mol	Joback Method
hfus	14.42	kJ/mol	Joback Method
hvap	39.84	kJ/mol	Joback Method
log10ws	-0.20		Crippen Method
logp	-0.029		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	409.51	K	Joback Method
tc	603.29	K	Joback Method
tf	256.08	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.59	J/mol×K	409.51	Joback Method

cpg	137.09	J/mol×K	441.81	Joback Method
cpg	143.29	J/mol×K	474.10	Joback Method
cpg	149.20	J/mol×K	506.40	Joback Method
cpg	154.83	J/mol×K	538.70	Joback Method
cpg	160.18	J/mol×K	570.99	Joback Method
cpg	165.26	J/mol×K	603.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.50 ± 1.50	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96300&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume